Clustering Mixtures with Almost Optimal Separation in Polynomial Time

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Joint work with Jerry Li (Microsoft Research)

(Gaussian) Mixture Models

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Mixture Models

Given a class of distributions $\mathcal{D}$, a mixture of k elements from $\mathcal{D}$ is a distribution of the form

$$\mathcal{M} = \sum_{i=1}^{k} w_i D_i \ ,$$

where $D_1, \ldots, D_k \in \mathcal{D}$, and w_i satisfy $w_i \geq 0$ and $\sum_{i=1}^{k} w_i = 1$.

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Mixture models and GMMs are well-studied theoretically, and popular in practice as a way to model heterogeneous data.

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Separation conditions

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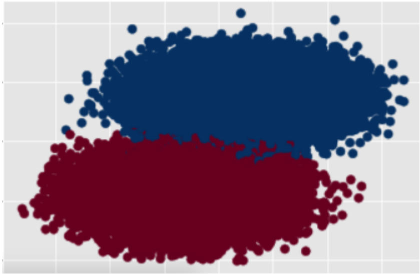
Need separation in TV-distance between components for clustering to be possible information-theoretically



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Main Question

What is the minimum Δ you need to *efficiently* cluster?

The information theoretic limit

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For simplicity, assume that mixing weights are uniform i.e. $w_i = 1/k$ for all $i = 1, \ldots, k$.

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Fact [Regev, Vijayaraghavan 2017]

$\Delta = \Theta(\sqrt{\log k})$ is both necessary and sufficient to obtain a clustering that is 99% accurate with high probability.

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Question

Can we cluster in polynomial time down to the information theoretic limit?

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Theorem

Let $c > 0$, and let $\mathcal{M}$ be a (uniform) mixture of isotropic Gaussians with separation $\Delta = \Omega(\log^{1/2+c} k)$. Then, there is an algorithm which takes $n = \mathrm{poly}(k, d)$ samples from $\mathcal{M}$ and runs in time $\mathrm{poly}(k, d)$, and which recovers a perfect clustering of the samples with high probability.

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- Our algorithm also works for non-uniform mixtures.
- We can also handle mixtures of shifts of any distribution D satisfying the Poincaré inequality under a mild additional condition

Outline

- **The barrier to existing approaches**
- Our techniques
  - Implicit Moment Estimation
  - Implicit Moment Computation
- Putting it all together

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2. If moments are distorted compared to those of a standard Gaussian then we can cluster
3. If separation between means is $\Omega(k^{\epsilon})$ then we need to measure moments of degree $1/\epsilon$ to detect distortions

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We develop new techniques for accessing/manipulating this information more efficiently

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- One component has mean 0
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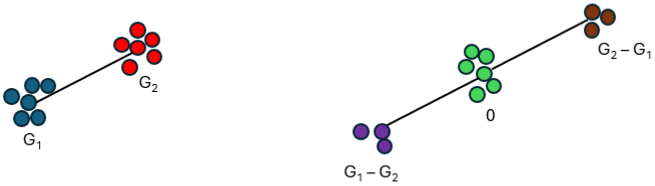

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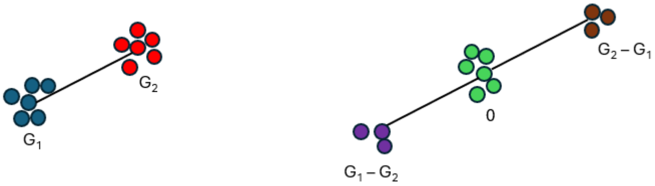

Let $\mathcal{M}$ be the difference mixture for the rest of this talk

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Let $X_1, \ldots, X_n$ be a set of polynomially many samples from $\mathcal{M}$. Given a new sample $X' \sim \mathcal{M}$, distinguish between the case where $X' \sim N(0, I)$, and $X' \sim N(\mu_i, I)$, for some $i \geq 1$.

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For simplicity, also assume that $\Delta = \mathrm{poly}(\log k)$, and $\|\mu_i\|_2 = \mathrm{poly}(\log k)$, for all i.

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Test function f will be a polynomial of degree t. The key will be to bound the variance.

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- It reliably witnesses large means, i.e. if $\|\mu\| \geq \Omega(t^{1/2})$ and $X \sim N(\mu, I)$, then with high probability,

$$\langle h_t(X), \mu^{\otimes t} \rangle \geq (0.8 \, \|\mu\|)^{2t} \geq \mathrm{poly}(k) \; .$$

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Issue: we only know that the variance of $h_t(X)$ in each direction is bounded but it has d^t entries which is too many

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Want Π to project onto $\mathrm{span}(\mu_1^{\otimes t}, \ldots, \mu_k^{\otimes t})$ - which is k-dimensional!

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Lemma: 0-component

Let $X \sim N(0, I)$. Then $\|\Pi_t h_t(X)\| \leq k^{1/2} \cdot O(t)^{t/2}$ with high probability.

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Lemma: 0-component

Let $X \sim N(0, I)$. Then $\|\Pi_t h_t(X)\| \leq k^{1/2} \cdot O(t)^{t/2}$ with high probability.

2. $f(X)$ is large with high probability if X is from a component with mean bounded away from 0

Lemma: Nonzero-component

Let $X \sim N(\mu_i, I)$, where $\|\mu_i\| \geq \Omega(t^{1/2})$. Then $\|\Pi_t h_t(X)\| \geq (0.8 \|\mu_i\|)^t$ with high probability.

Verifying Soundness

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Takeaway: if we know $\Pi_t = \text{span}(\mu_1^{\otimes t}, \ldots, \mu_k^{\otimes t})$ then we can cluster with polynomially many samples

Outline

- The barrier to existing approaches
- **Our techniques**
  - Implicit Moment Estimation
  - **Implicit Moment Computation**
- Putting it all together

Important Ingredients

1. Estimating degree $t = \Theta(\log k / \log \log k)$ moments accurately
   - We show certain projections of the moment tensor have *polynomially bounded variance*
   - We can estimate these projections *sample-efficiently*

2. **Representing the degree $t = \Theta(\log k / \log \log k)$ moment tensor efficiently**
   - We only need to perform a restricted set of operations on the moment tensor
   - These can be *performed implicitly in polynomial time*

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- **Main idea:** we construct such a representation inductively (in t)

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Preview

- **Main idea:** we construct such a representation inductively (in t)
- $\Pi_t : \mathbb{R}^{d^t} \to \mathbb{R}^k$ is too large to write down – we will compute an implicit representation of Π_t that has polynomial size and allows us to perform certain restricted operations in polynomial time

Iterative projection maps

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Inductive Step: Let $\Pi_{s-1} = \text{span}\left(\mu_1^{\otimes(s-1)}, \ldots, \mu_k^{\otimes(s-1)}\right)$

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Goal: Construct a representation of $\Pi_s = \text{span}\left(\mu_1^{\otimes s}, \ldots, \mu_k^{\otimes s}\right)$

Constructing the Projection (cont.)

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Given samples $X_1, \ldots, X_n \sim \mathcal{M}$, estimate

$$\frac{1}{n}\sum_{i=1}^{n} h_{2s}(X_i) \approx \mathop{\mathbb{E}}_{X\sim\mathcal{M}}[h_{2s}(X)] = \sum_{i=1}^{k} w_i \mu_i^{\otimes 2s} .$$

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If we treat this as a $d^s \times d^s$ matrix, we can write this as

$$T_{2s} = \sum_{i=1}^{k} w_i \left(\mu_i^{\otimes s}\right)\left(\mu_i^{\otimes s}\right)^{\top} .$$

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This matrix is too large to work with, but we can make use of the inductive step

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Define the projection matrix

$$B_s = I_{d \times d} \otimes \Pi_{s-1} : \mathbb{R}^{d^s} \to \mathbb{R}^{dk} \ .$$

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We set $\Pi_s = \Gamma_s B_s$

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Claim: $\text{span}\left(\mu_1^{\otimes s}, \ldots, \mu_k^{\otimes s}\right) = \Gamma_s B_s$.

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Claim: $\text{span}\left(\mu_1^{\otimes s}, \ldots, \mu_k^{\otimes s}\right) = \Gamma_s B_s$.
Proof: It suffices to check that $\Gamma_s B_s$ preserves the norm of all $\mu_i^{\otimes s}$.

$$\begin{aligned} \left\| \Gamma_s B_s \mu_i^{\otimes s} \right\| &= \left\| B_s \mu_i^{\otimes s} \right\| \\ &= \left\| \mu_i \otimes \Pi_{s-1} \mu_i^{\otimes(s-1)} \right\| \\ &= \| \mu_i \| \left\| \Pi_{s-1} \mu_i^{\otimes(s-1)} \right\| = \| \mu_i \|^s \ . \end{aligned}$$

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4. Output $\Pi_s = \Gamma_s B_s$.

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Key Fact: $\Pi_s v$ can be computed efficiently on rank-1 tensors i.e. of the form $v = v_1 \otimes \cdots \otimes v_s$ because

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We can (only) efficiently apply the projection to rank-1 tensors

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Want to show: To evaluate $\Pi_t h_t(X)$, we need to represent $h_t(x)$ as a low-rank tensor!

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We view $R_t(X)$ as a polynomial with random coefficients

Low rank approximations of Hermite polynomials (cont.)

Lemma

For all t, there is a (random) polynomial $R_t : \mathbb{R}^d \to \mathbb{R}^{d^t}$ satisfying:

- **Unbiased:** *For all $X \in \mathbb{R}^d$, we have*

$$\mathop{\mathbb{E}}_{R_t}[R_t(X)] = h_t(X) \ .$$

- **Bounded Variance:** *For all $v \in \mathbb{R}^{d^t}$ with $\|v\| = 1$, we have*

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- **Low Rank:** *R_t can always be written as a sum of $\mathrm{poly}(k)$ many (explicit) rank-1 tensors.*

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Proof: See paper...

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4. If $\alpha < k^{1/2} O(t)^{t/2}$, say that X' belongs to the 0 mean cluster, otherwise, say it belongs to a non-zero mean cluster.

Generalizing to Poincaré

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A distribution is σ-Poincaré if

$$\mathrm{Var}[f(X)] \leq \sigma^2 \, \mathbb{E}\left[\|\nabla f(X)\|^2\right] \; .$$

Well studied class of distributions, including Gaussians, product distributions, and log-concave distributions (thanks to KLS).

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Our techniques generalize almost directly to Poincaré distributions, by using *adjusted* polynomials in place of Hermite polynomials.

Here, we require separation $\Delta = \Theta(\log^{1+c} k)$, but this is information-theoretically necessary, since Poincaré distributions could have worse concentration.

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To circumvent this and obtain a perfect clustering, we exploit the structure of Gaussians to recursively cluster

- It is not clear how to do this recursion for general Poincaré distributions.

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Thanks!